Butanoic acid, 2-chloro, 1,1-dimethylethyl ester

Inchi: InChI=1S/C8H15ClO2/c1-5-6(9)7(10)11-8(2,3)4/h6H,5H2,1-4H3
InchiKey: VAUWEPUIEVLFSB-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CCC(Cl)C(=O)OC(C)(C)C
Mol. weight [g/mol]: 178.66

Physical Properties

Property code	Value	Unit	Source
gf	-228.97	kJ/mol	Joback Method
hf	-483.02	kJ/mol	Joback Method
hfus	12.52	kJ/mol	Joback Method
hvap	45.26	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.345		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1012.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1003.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1287.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1299.00		NIST Webbook
tb	492.49	K	Joback Method
tc	688.63	K	Joback Method
tf	269.42	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.00	J/mol×K	492.49	Joback Method

cpg	324.20	J/mol×K	525.18	Joback Method
cpg	336.72	J/mol×K	557.87	Joback Method
cpg	348.58	J/mol×K	590.56	Joback Method
cpg	359.80	J/mol×K	623.25	Joback Method
cpg	370.40	J/mol×K	655.94	Joback Method
cpg	380.41	J/mol×K	688.63	Joback Method
dvisc	0.0057226	Pa×s	269.42	Joback Method
dvisc	0.0024535	Pa×s	306.60	Joback Method
dvisc	0.0012634	Pa×s	343.78	Joback Method
dvisc	0.0007405	Pa×s	380.96	Joback Method
dvisc	0.0004773	Pa×s	418.13	Joback Method
dvisc	0.0003305	Pa×s	455.31	Joback Method
dvisc	0.0002420	Pa×s	492.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28540&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume